8 On QED

8.1 Introduction

Underpinning the Dirac-level theory we have *quantum electrodynamics*, QED. It is the theory on virtual photon processes. The two simplest terms are denoted by the **Feynman** diagrams

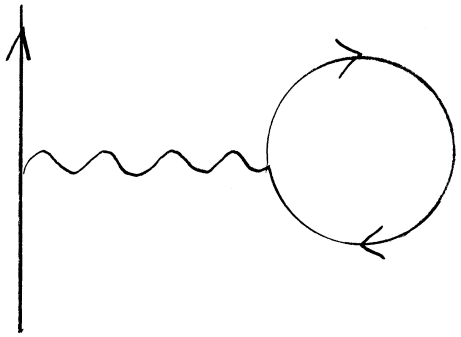

Figure 8.1: Vacuum polarization

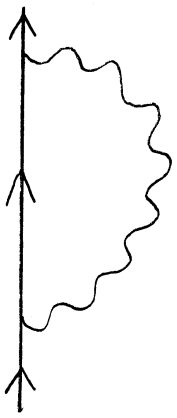

Figure 8.2: Self-energy

The lowest-order *vacuum polarization* (VP) term can be expressed in analytical form (**Uehling** 1935). It is independent of the nuclear charge, a property of the vacuum. Furthermore, it is attractive. The *self energy* (SE) is larger than the VP and of opposite sign. Both can be related (to lowest order) to $|\Psi(0)|^2$. The QED is a *covariant* theory.

8.2 Some formulas for vacuum polarization

$$V_n^{\text{eff}}(r) = -\frac{Z}{r}(1 + S(r)) = V_n + V_{\text{Ue}}, \tag{8.1}$$

$$S(r) = \frac{2\alpha}{3\pi}\int_1^\infty \exp\Big(-\frac{2r\chi}{\alpha}\Big)\Big(1+\frac{1}{\chi^2}\Big)\frac{\sqrt{\chi^2-1}}{\chi^2}d\chi \tag{8.2}$$

The Uehling function $S(r)$ can be fitted to the two-parameter expression

$$\begin{aligned} S(r) = \alpha\Big[&\exp(-d_1 r^2)C_1\left[\ln(\alpha/r) - C_2\right] \\ &+(1-\exp(-d_1 r^2))\Big(\frac{1}{C_3}\Big)\frac{\exp(-2r/\alpha)}{d_2(\frac{r}{\alpha})^{0.5}+(\frac{r}{\alpha})^{1.5}}\Big] \end{aligned} \tag{8.3}$$

Here the free parameters $d_1 = 0.678 \cdot 10^7$ and $d_2 = 1.4302$. The three constants are

$$C_1 = \frac{2}{2\pi}, \quad C_2 = \frac{5}{6} + C, \quad C_3 = 4\sqrt{\pi} \tag{8.4}$$

Also see figure (8.3).

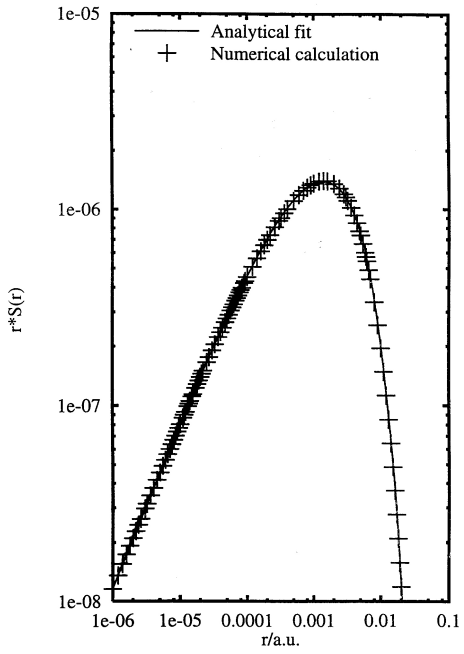

Figure 8.3: The Uehling function $rS(r)$

8.3 Some formulas for self-energy (vacuum fluctuation)

For light elements one can use the *density formula*

$$E_{\rm SE} = \frac{4Z\alpha^3}{3}\left[\ln\frac{1}{(\alpha Z)^2} - \ln\frac{2K_{n0}}{(\alpha Z)^2} + \frac{5}{6}\right]|\Psi(0)|^2 \tag{8.5}$$

Alternatively the total *Lamb shift* is obtained to lowest order from the density as

$$E_{\rm L} = \frac{4Z\alpha^3}{3}\left[\ln\frac{1}{(\alpha Z)^2} - \ln\frac{2K_{n0}}{(\alpha Z)^2} + \frac{19}{30}\right]|\Psi(0)|^2 \tag{8.6}$$

For heavy elements, evaluate $E_{\rm SE}$ from the $2s$ SE/VP ratio of **Johnson** and **Soff** (1985), The total valence-electron Lamb shift becomes

$$E_{\rm L} = \langle V_{\rm Ue}\rangle \frac{(E_{\rm SE} + E_{\rm VP})}{E_{\rm VP}} \tag{8.7}$$

For the valence electrons the order-of-magnitude of the Lamb shift remained unknown, beyond lithium, until the two papers

[1] P. Pyykkö, M. Tokman, L.N. Labzowsky, *Phys. Rev. A* **57** (1998) R 689

[2] L. Labzowsky, I. Goidenko, M. Tokman, P. Pyykkö, *Phys. Rev. A* **59** (1999) 2707

[1] used the density-based or the "ratio" methods. It also introduced a semiempirical "A-model" ('A' for the nuclear A-value). In [2], using spline-functions in a local model potential, the Feynman diagrams were actually calculated for the ns valence electrons of alkali and coinage metals. The results were very similar: For $Z \gtrapprox 50$, the Lamb shift is about -1% of the Dirac-level effects. Figures (8.4) and (8.5) give an idea of the size of the effects.

For lighter elements it is, relatively speaking, larger. A simple way to estimate it is to scale the Darwin term, as suggested in

[3] P. Pyykkö, K.G. Dyall, A.G. Császár, G. Tarczay, O.L. Polyansky and J. Tennyson, *Phys. Rev. A* **63** (2001), 024502, 1-4

$$E^{\rm Lamb}/E^{\rm Darwin} = \frac{8\alpha}{3\pi}\big[-2\ln(\alpha Z) - \ln X + \frac{19}{30}\big] \tag{8.8}$$

$$E^{\rm Lamb}/E^{\rm Darwin} = \frac{2\alpha F(Z\alpha)}{\pi} - \frac{8\alpha}{15\pi} \tag{8.9}$$

$$E^{\rm Lamb}/E^{\rm Darwin} = \frac{8\alpha}{3\pi}\ln(\frac{1}{Z\alpha}) \tag{8.10}$$

Equation (8.10) was introduced by **Bjorken** and **Drell** (1964). The results of using the above three equations can be studied in figure (8.6).

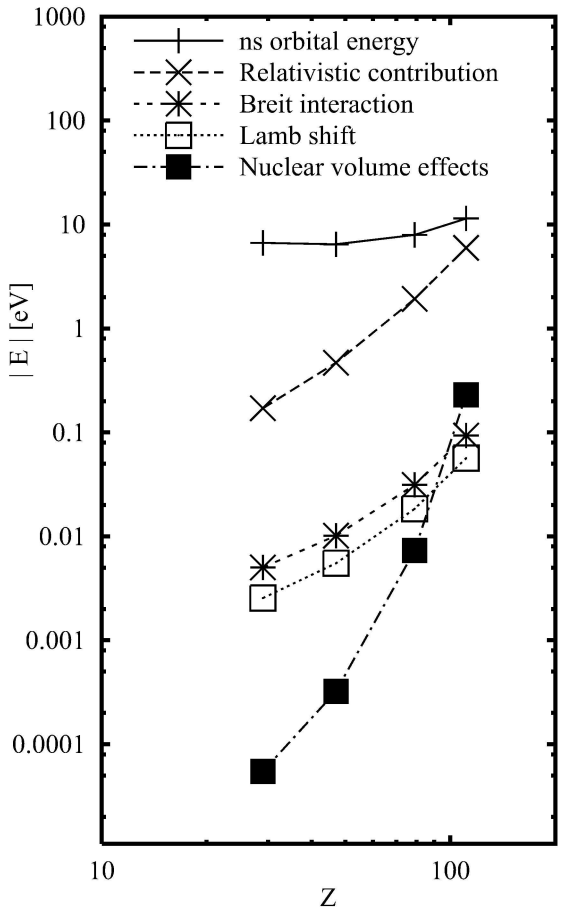

Figure 8.4: Dirac-Fock contributions for coinage metals. From P. Pyykkö, M. Tokman and L.N. Labzowsky, *Phys. Rev. A* **57** (1998) R689

Recall the Pauli Hamiltonian

$$h_p = -\frac{\alpha^2}{8}\underset{\sim}{p}^4 - \frac{\alpha^2}{8}\nabla^2 V - \frac{\alpha^2}{4}\underset{\sim}{\sigma}\cdot(\nabla V \times \underset{\sim}{p}) \tag{8.11}$$

where for a Coulomb potential

$$\nabla^2 V = -4Z\pi\delta(\underset{\sim}{r}) \tag{8.12}$$

X is related to the **Bethe logarithm** K_{n0}:

$$X = 2K_{n0}/(\alpha Z)^2 \;\approx\; 11.77, 16.64, 15.93, \ldots \quad \text{for 1s, 2s, 3s, } \ldots \tag{8.13}$$

The $F(\alpha Z)$ is used to express the exact self energy as

$$E_1^{\mathrm{SE}} = \alpha^3 Z F(\alpha Z)\langle\delta(\underset{\sim}{r})\rangle \tag{8.14}$$

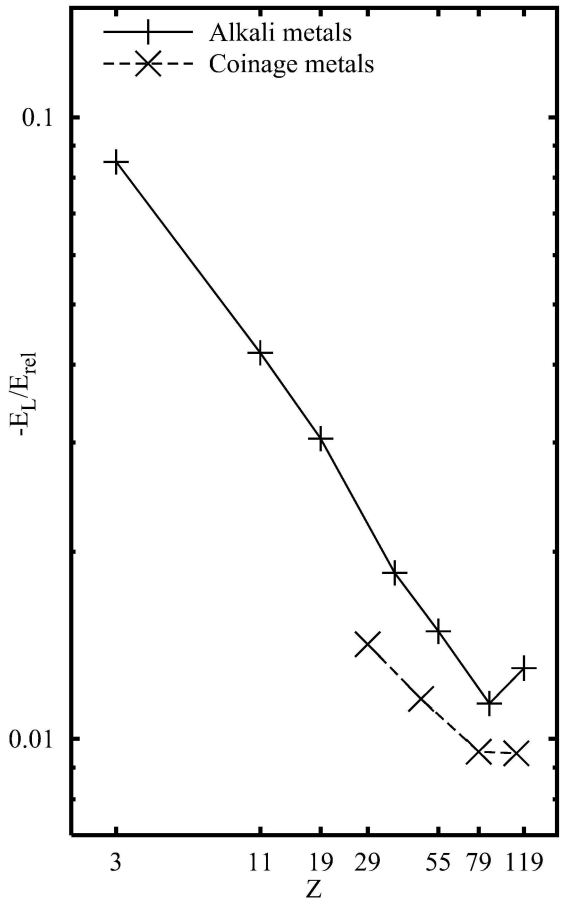

Figure 8.5: Ratios of the Lamb shift to the relativistic contribution. From L. Labzowsky, I. Goidenko, M. Tokman, P. Pyykkö, *Phys. Rev. A* **59** (1999) 2707

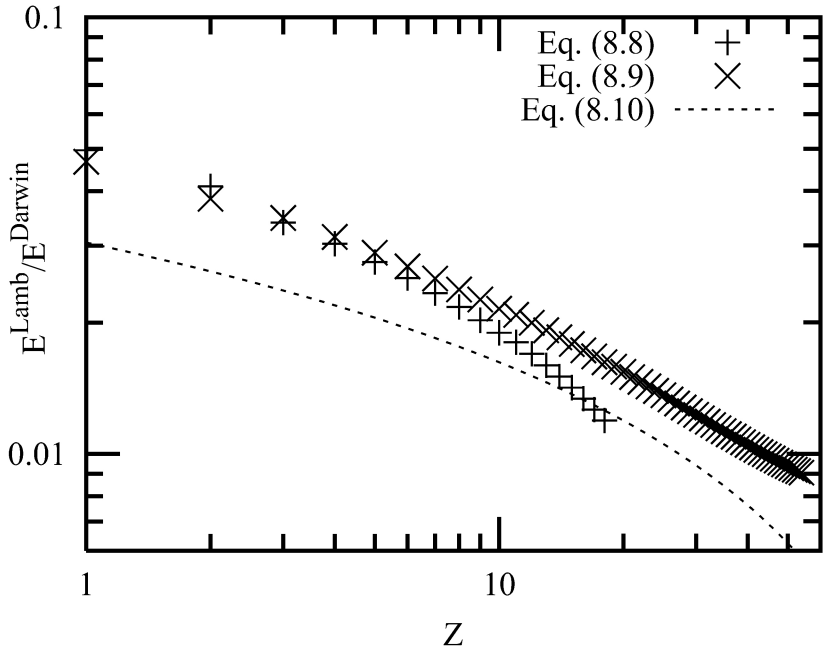

Figure 8.6: The ratio $E^{\mathrm{Lamb}}/E^{\mathrm{Darwin}}$. From P. Pyykkö *et al.* , *Phys. Rev. A* **63** (2001), 024502, 1-4

	$1S_{1/2}$
Binding energy E_B (point nucleus)	**-93459.89**
Corrections:	
Finite nuclear size	49.13
Self energy (order α)	196.68
VP: Uehling contribution	*-41.99*
VP: Wichmann-Kroll contribution	*1.79*
Total vacuum polarization (order α)	-40.20
SESE (2^{nd} order SE) (a) (b) (c)	
VPVP (2^{nd} order VP) (a) (ladder diagrams)	-0.07
VPVP (b) (Källén-Sabry contribution + h.o.)	-0.05
VPVP (c) (Källén-Sabry contribution)	-0.29
SEVP (a) (b) (c)	0.42
S(VP)E	0.05
Radiative recoil (estimate)	*0.00*
Reduced mass	*0.26*
Relativistic recoil	*0.08*
Total recoil	0.34
Nuclear polarization (*bottleneck for accuracy!*)	-0.02
Sum of corrections	205.99
Resulting total binding energy	**-93253.90**
Lamb shift (theory)	**205.73**
(experimental)	**202(8)**

Figure 8.7: One-electron Lamb shift contributions for $^{197}Au^{78+}$ (hydrogen-like gold). Energy values are given in eV. From T. Beier *et al.*, *Phys. Lett. A* **236** (1997) 329-338